UK Atomic Energy Authority

An algorithmic framework for developing saturation rules in reduced core transport models

H.G. Dudding[*,1] F.J. Casson[1], D. Dickinson[2], B.S. Patel[1], C.M. Roach[1], E.A. Belli[3], G.M. Staebler[4]

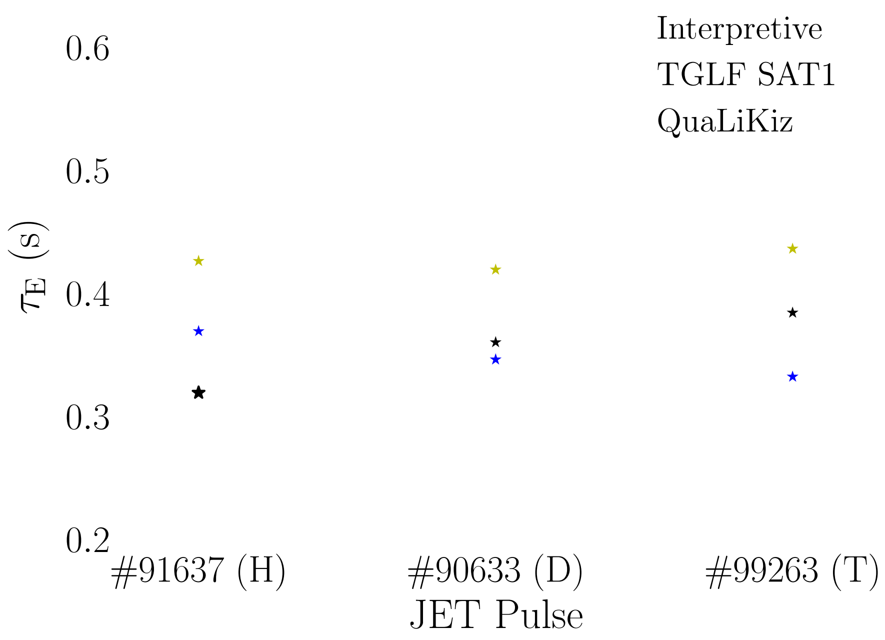
*Email: harry.dudding@ukaea.uk
[1]Culham Centre for Fusion Energy, Abingdon, Oxfordshire, OX14 3DB, UK
[2] Department of Physics, York Plasma Institute, University of York, Heslington, York YO10 5DD, United Kingdom
[3] General Atomics, San Diego, CA 92186-5608, United States of America
[4]Oak Ridge National Laboratory, Oak Ridge, TN 37830, United States of America

Introduction

- Reduced turbulence models are needed for integrated modelling due to relatively low computational expense

- Quasilinear (QL) models (TGLF, QuaLiKiz) approximate fluxes using *simplified* linear physics and a **saturation rule**

- Saturation rules built from theory and fits to NL GK simulations
  $\Longrightarrow$ can extrapolate poorly to new parameter space



TGLF: G.M. Staebler *et al* 2007 *Phys. Plasmas* **14** 055909
QuaLiKiz: C. Bourdelle *et al* 2016 *Plasma Phys. Control. Fusion* **58** 014036

Introduction

UK Atomic Energy Authority

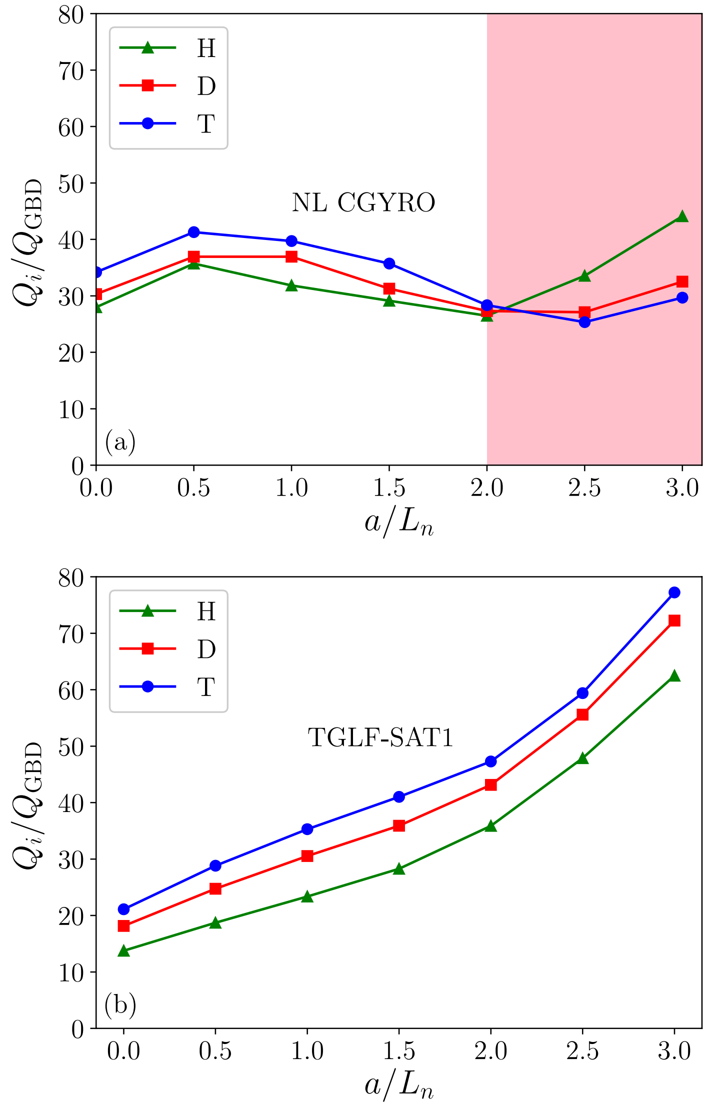
- Typically tuned on **large aspect-ratio**, **electrostatic**, **deuterium** plasmas

- We require *validated* transport models for current and future experiments, particularly in areas of e.g:

• Fast ions	• Mixed plasmas
• Plasma shaping	• Electromagnetic turbulence/ High β

- Test models via comparison with standalone NL GK simulations

- In this talk, focus on the development of the new saturation rule SAT3 from discrepancies in **isotope scaling**



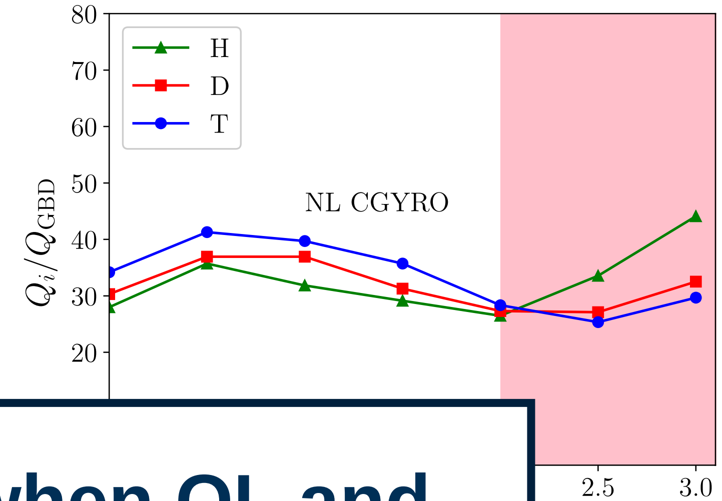
Introduction

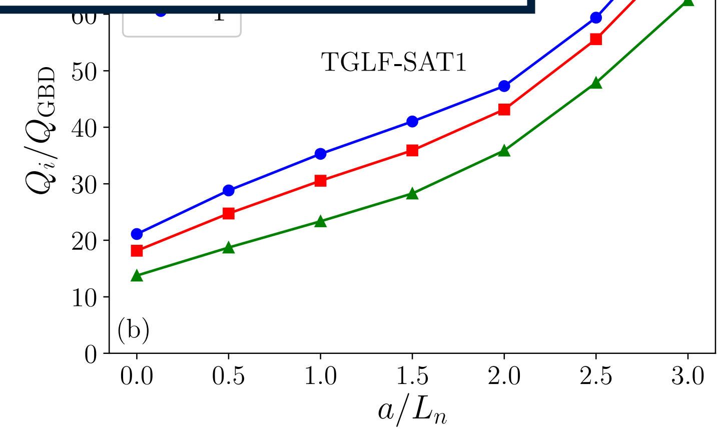
- Typically tuned on **large aspect-ratio**, **electrostatic**, **deuterium** plasmas

- We require *validated* transport models for current and future experiments, particularly in areas of e.g:

  - Fast io
  - Plasma shaping

What do we do when QL and NL GK don't agree?





- Test models via comparison with standalone NL GK simulations

- In this talk, focus on the development of the new saturation rule SAT3 from discrepancies in **isotope scaling**

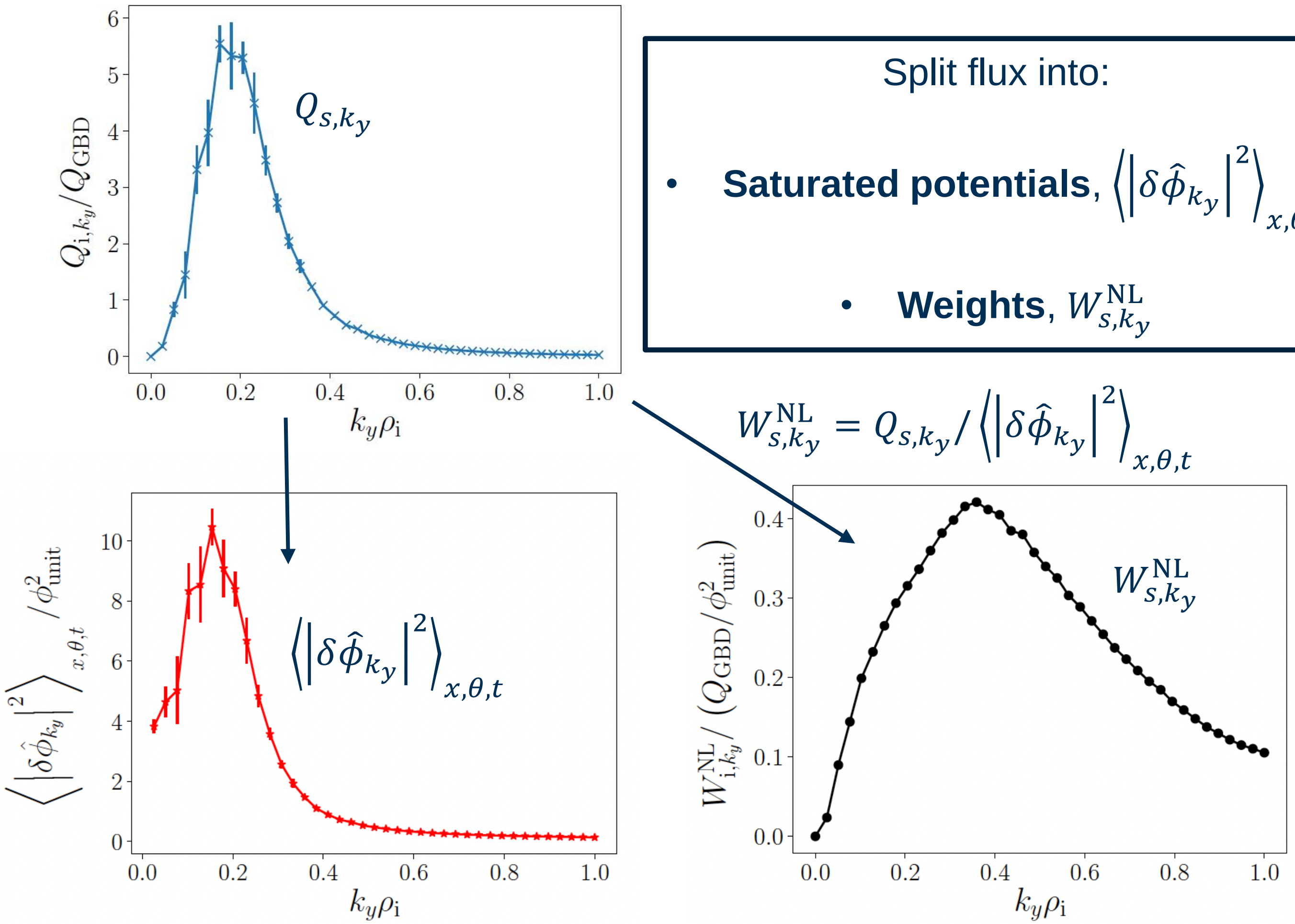
Turbulent flux theory

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$

Split flux into:

- **Saturated potentials**, $\left\langle \left|\delta\hat{\phi}_{k_y}\right|^2 \right\rangle_{x,\theta,t}$
- **Weights**, W^{NL}_{s,k_y}

$$W^{\mathrm{NL}}_{s,k_y} = Q_{s,k_y} / \left\langle \left|\delta\hat{\phi}_{k_y}\right|^2 \right\rangle_{x,\theta,t}$$



Turbulent flux theory

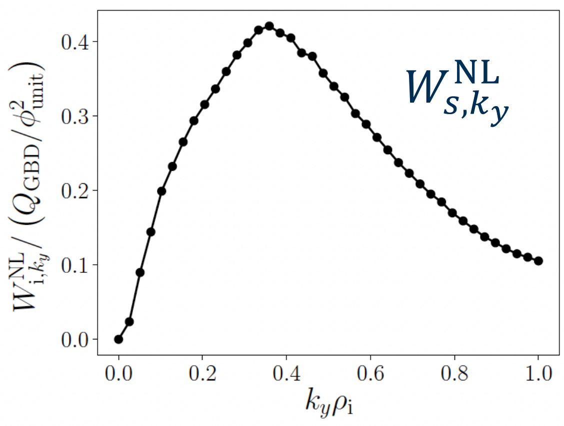
$$Q_s = \sum_{k_y > 0} Q_{s,k_y}$$

$$= \sum_{k_y > 0} W_{s,k_y}^{\mathrm{NL}} \left\langle \left| \delta \hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

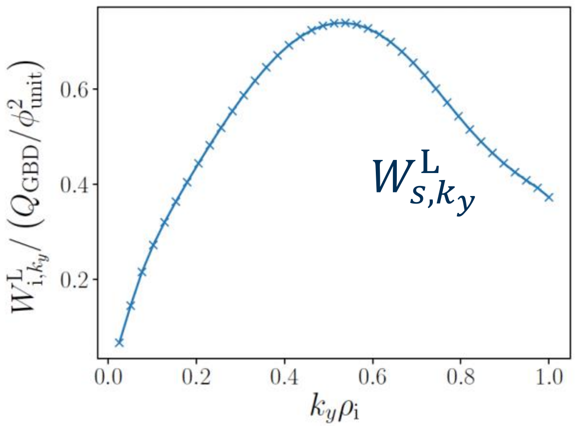
Turbulent flux theory: The quasilinear approximation

- W^{NL}_{s,k_y} calculated from **saturated** turbulence in **nonlinear** simulation
- Can also calculate the phase difference in a **linear** simulation, W^{L}_{s,k_y}

'The quasilinear approximation': $W^{\mathrm{NL}}_{s,k_y} \approx W^{\mathrm{L}}_{s,k_y}$



$\approx$



- Quantify departure from perfect agreement via $W^{\mathrm{NL}}_{s,k_y} = \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y}$

Turbulent flux theory

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$

$$= \sum_{k_y>0} W^{\mathrm{NL}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

$$= \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

Turbulent flux theory

UK Atomic Energy Authority

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$

$$= \sum_{k_y>0} W^{\mathrm{NL}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

$$= \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

Quasilinear models:

Turbulent flux theory

UK Atomic Energy Authority

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$

$$= \sum_{k_y>0} W^{\mathrm{NL}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

$$= \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

Quasilinear models:

Λ_{s,k_y}: Assume $\approx const.$
(QL approximation)

Turbulent flux theory

UK Atomic Energy Authority

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$

$$= \sum_{k_y>0} W^{\mathrm{NL}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

$$= \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

Quasilinear models:

Λ_{s,k_y}: Assume $\approx const.$ (QL approximation)

W^{L}_{s,k_y}: Approximate using *simplified* linear solver

Turbulent flux theory

UK Atomic Energy Authority

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$

$$= \sum_{k_y>0} W^{\mathrm{NL}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

$$= \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

Quasilinear models:

Λ_{s,k_y}: Assume $\approx const.$ (QL approximation)

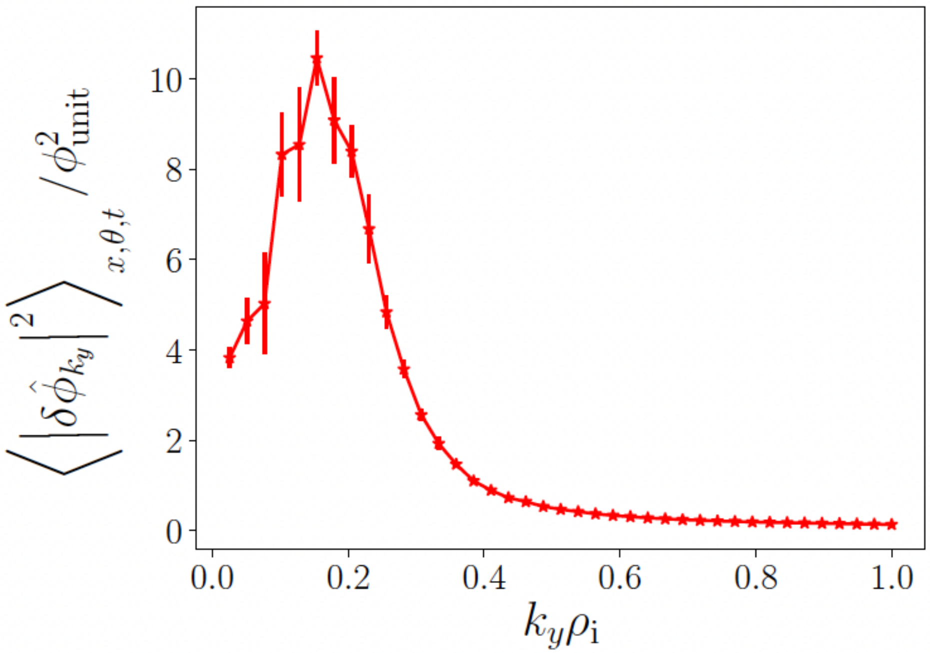
W^{L}_{s,k_y}: Approximate using *simplified* linear solver

$\left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$: Approximate using **saturation rule**

Saturation Rules

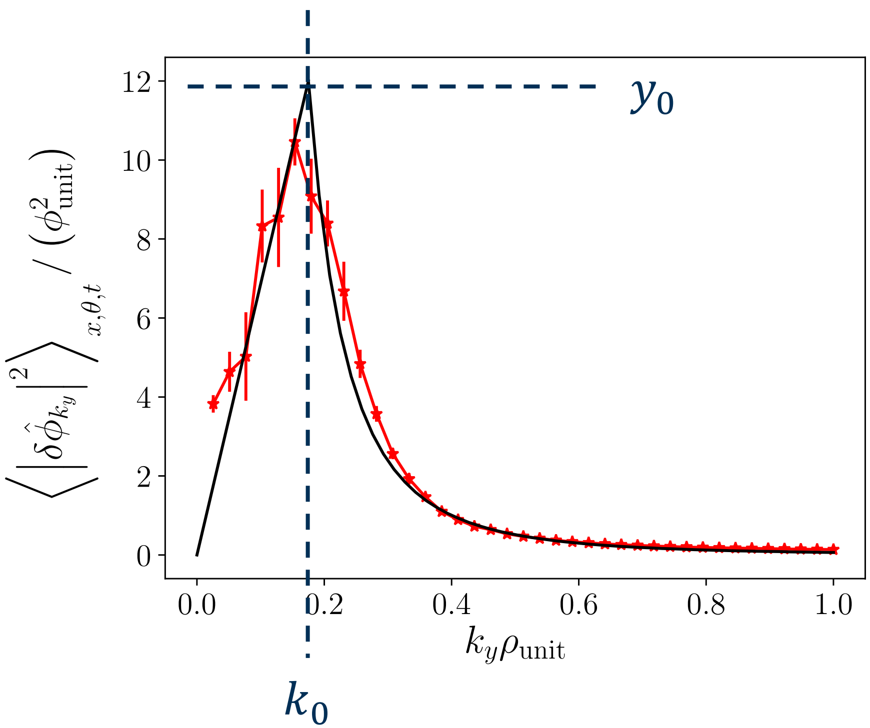
- Saturation **inherently nonlinear** process $\Longrightarrow$ cannot invoke linear gyrokinetics like with the weights

- Saturation rules guided by theory and fits to NL GK data to predict potential spectra



Saturation Rules: QLK example

$$y(k_y) = \begin{cases} y_0 \left({}^{k_y}\!/_{k_0} \right) & 0 < k_y \leq k_0 \\ y_0 \left({}^{k_y}\!/_{k_0} \right)^{-3} & k_0 < k_y < \infty \end{cases}$$



$$y(k_y) = y_0 S(k_y)$$

$S(k_y)$: **'Spectral shape'**

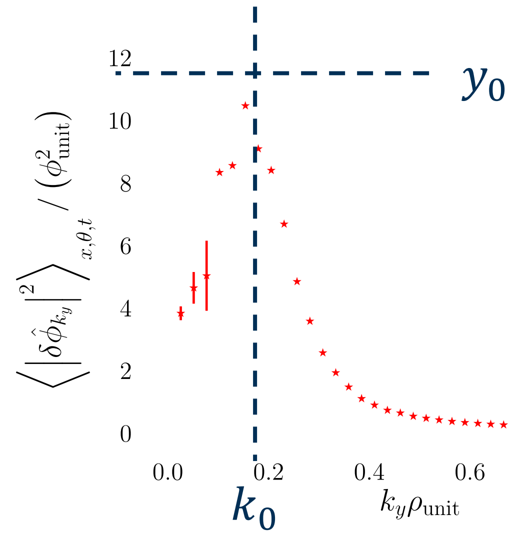
y_0: **'Saturation level'**

Still need to model y_0, k_0!

Saturation rules: linear modelling

- Parameters vary case-by-case ⟹ require ‘linear model’ for each one

- Use physics arguments to relate parameters to linear properties, e.g.

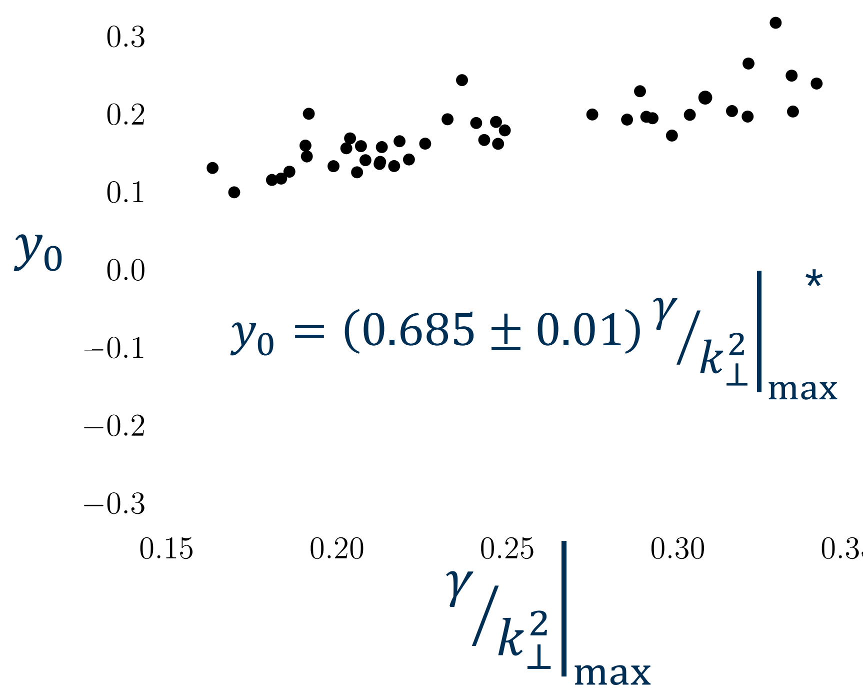


Mixing length rule

- Consider transport as *diffusive* process

- Argue that potential peak varies with diffusion coefficient

$$y_0 \sim D_\perp \sim \frac{\Delta l^2}{\Delta t} \propto \left.\frac{\gamma}{k_\perp^2}\right|_{\max}$$



- Recommended to fit using linear gyrokinetics, **not** simplified linear solvers

*Note: Toy data for illustrative purposes

Discrepancy algorithm

$$Q_s = \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

UK Atomic Energy Authority

Consider each aspect in turn, develop where necessary:

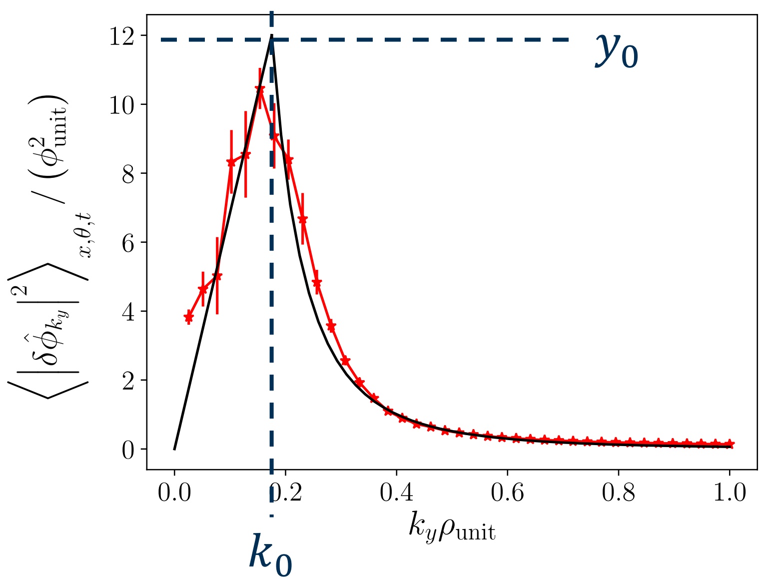
$\Lambda_{s,k_y} \approx const.$ valid?

W^{L}_{s,k_y} well-modelled by simplified linear solver?

Test spectral shape:
Sat. rule works well when parameters (e.g. y_0, k_0) fitted to NL GK data?

Test linear models:
Sat. rule works well when linear modelling done with linear GK?

$\Longrightarrow$ Inaccuracy of simplified linear solver distorting sat. rule



Addressing isotope scaling in TGLF

$$Q_s = \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

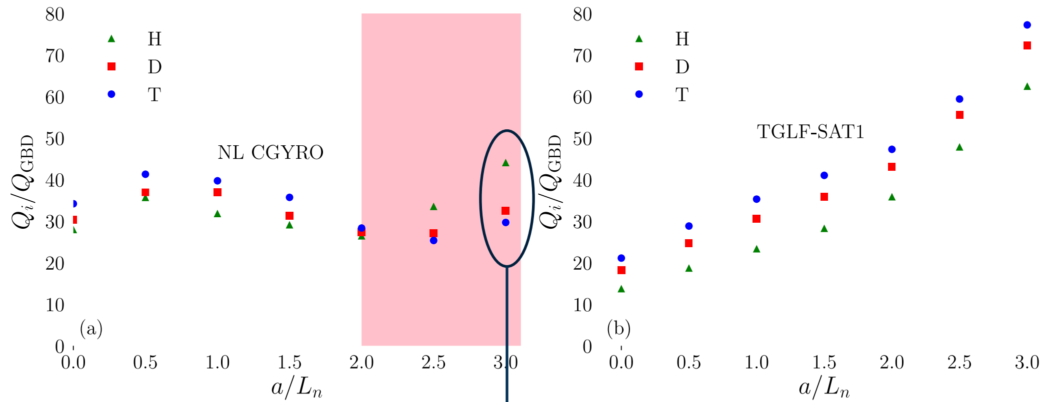
- Discrepancy between **isotope scaling** of fluxes in TEM-dominant regime

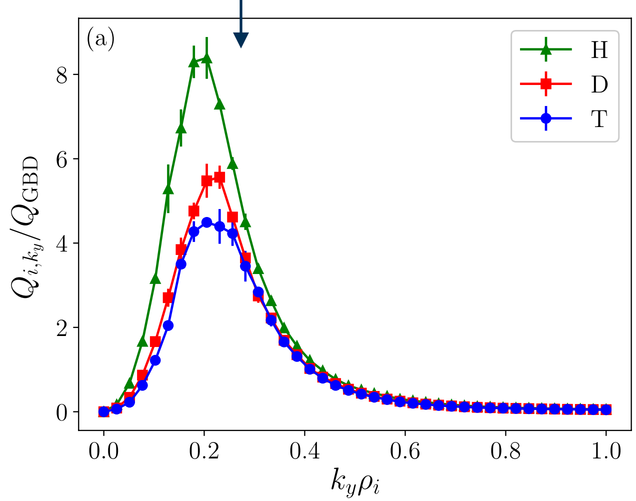
- $\Longrightarrow$ Build NL GK database of ~50 simulations, expanding on previous to include different isotopes (H, D, T)

- Begin discrepancy algorithm, find isotope scaling to originate in region of *low* k_y

- Found $\Lambda_{s,k_y} \approx const.$ and modelling of W^{L}_{s,k_y} to be well-satisfied

  $\Longrightarrow$ Turn to the saturation rule!



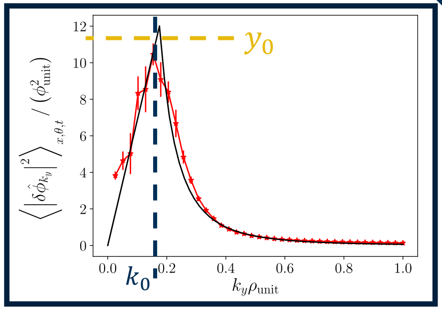


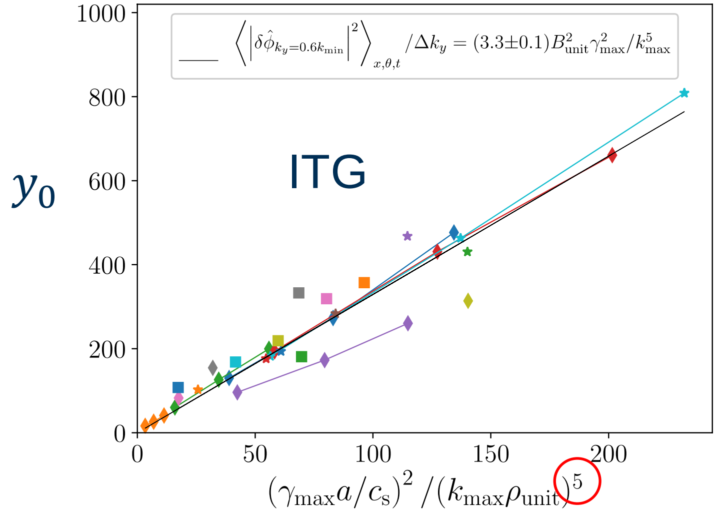
Addressing isotope scaling in TGLF: SAT3

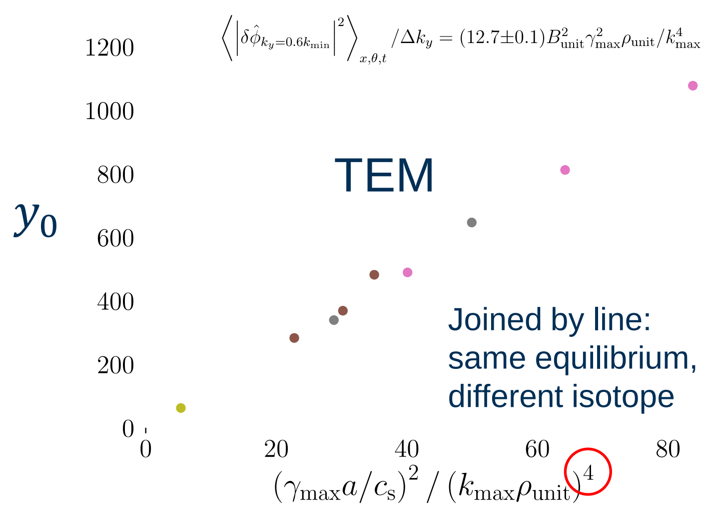
UK Atomic Energy Authority

$$Q_s = \sum_{k_y>0} \Lambda_{s,k_y} W^{\mathrm{L}}_{s,k_y} \left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}$$

- **Found dominant cause of isotope scaling to be linear modelling of the saturation level, y_0**
- Find **different** saturation levels depending on if turbulence is ITG or TEM-dominated
- SAT3 model allows for **transitioning** between saturation levels **depending** on dominant mode type

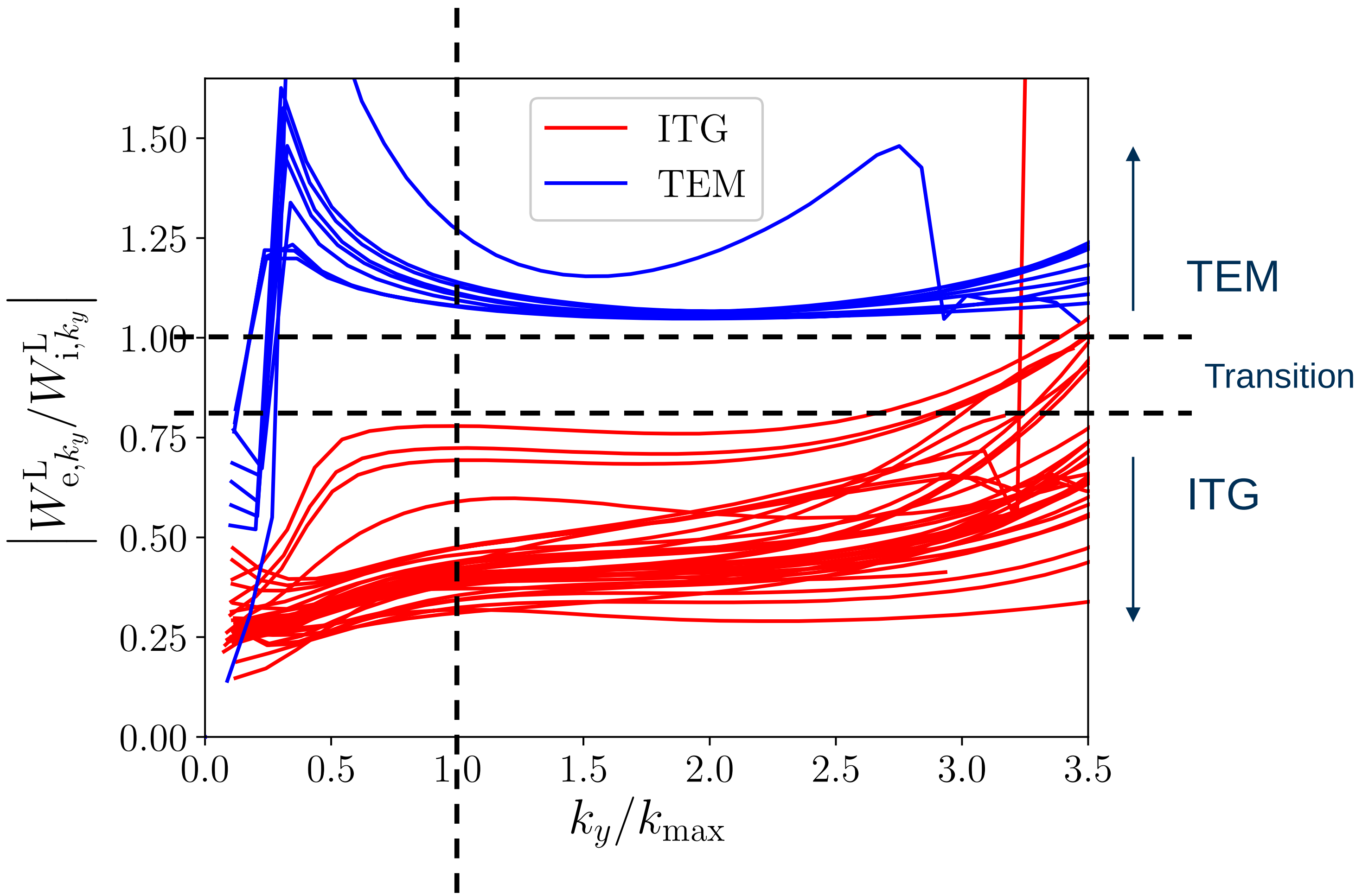






H.G. Dudding *et al* 2022 *Nucl. Fusion* **62** 096005

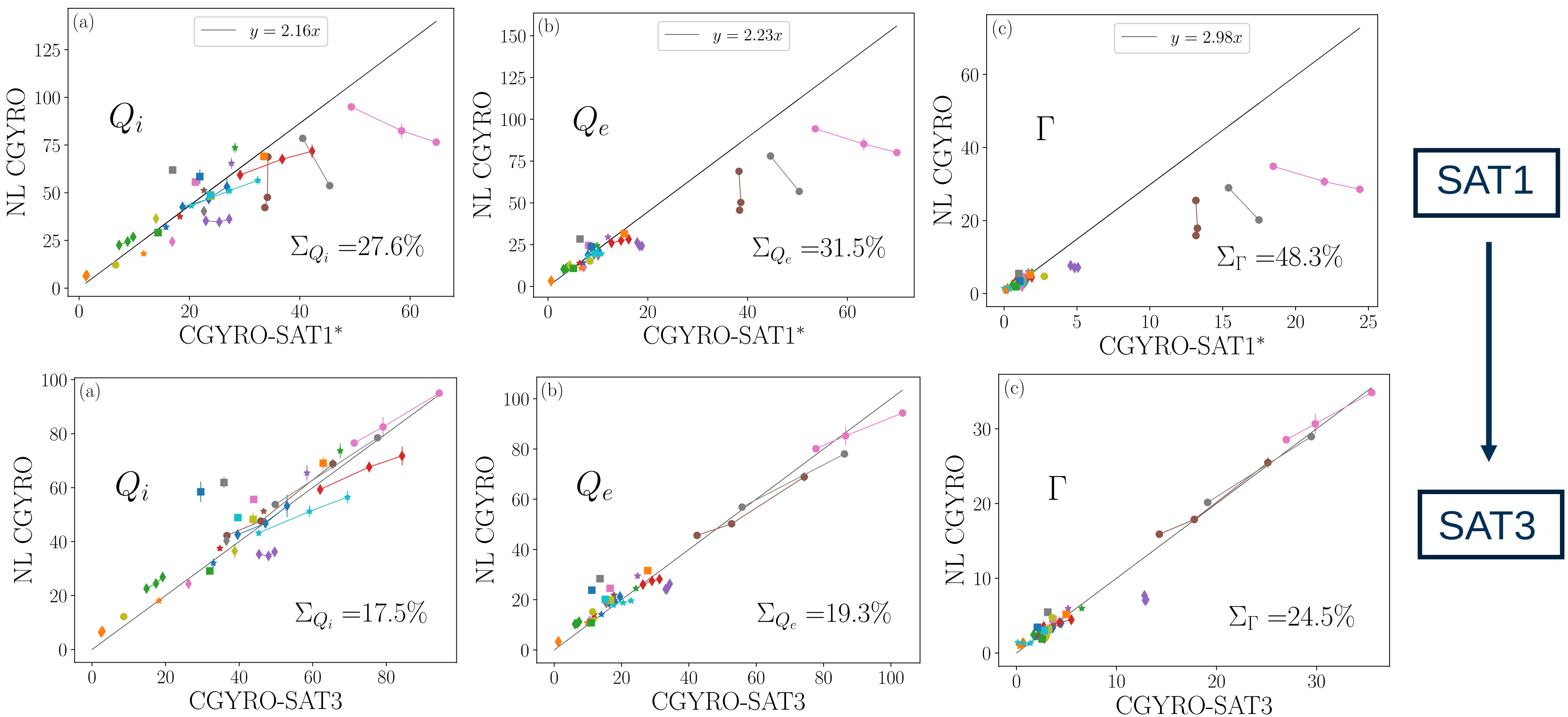
SAT3 mode identification



Addressing isotope scaling in TGLF: SAT3

UK Atomic Energy Authority

- These improvements allow us to capture the isotope scaling of TEM turbulence
- Constitutes **extension** of model validity while still performing well in established parameter spaces
- SAT3 available for use on GACODE master branch



SAT3/TEM-effect currently being validated in integrated modelling

Summary

UK Atomic Energy Authority

- Quasilinear transport models can perform less-well outside of their tuned parameter space

- Presented an algorithm to address discrepancies, focusing on the separation of each contribution to isolate the root cause

- Algorithm was applied in the development of SAT3, allowing us to correctly model the isotope scaling of TEM turbulence in QL models

- Integrated modelling validation efforts currently being performed

Discussion: future

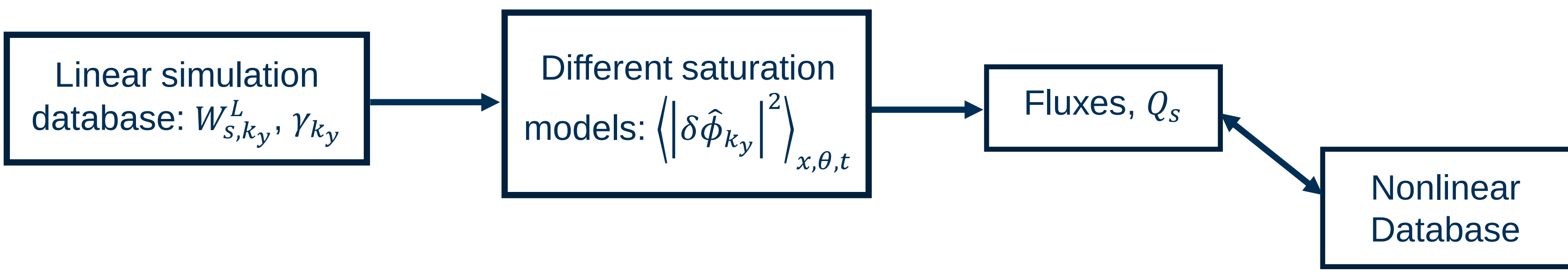
1. Electromagnetic fluxes:
   - 5 Λ_{s,k_y}-like quantities, 5 W^{L}_{s,k_y} -like quantities, 1 saturation rule
   - $\Longrightarrow$ Generalise first two steps of the algorithm

$$Q_s = \sum_{k_y>0} Q^{\delta\phi}_{s,k_y} + Q^{\delta A_{||}}_{s,k_y} + Q^{\delta B_{||}}_{s,k_y}$$

$$= \sum_{k_y>0} \left[\frac{Q^{\delta\phi}_{s,k_y}}{\left\langle\left|\delta\hat{\phi}_{k_y}\right|^2\right\rangle}\right]\left\langle\left|\delta\hat{\phi}_{k_y}\right|^2\right\rangle + \left[\frac{Q^{\delta A_{||}}_{s,k_y}}{\left\langle\left|\delta\hat{A}_{||,k_y}\right|^2\right\rangle}\right]\left\langle\left|\delta\hat{A}_{||,k_y}\right|^2\right\rangle + \left[\frac{Q^{\delta B_{||}}_{s,k_y}}{\left\langle\left|\delta\hat{B}_{||,k_y}\right|^2\right\rangle}\right]\left\langle\left|\delta\hat{B}_{||,k_y}\right|^2\right\rangle$$

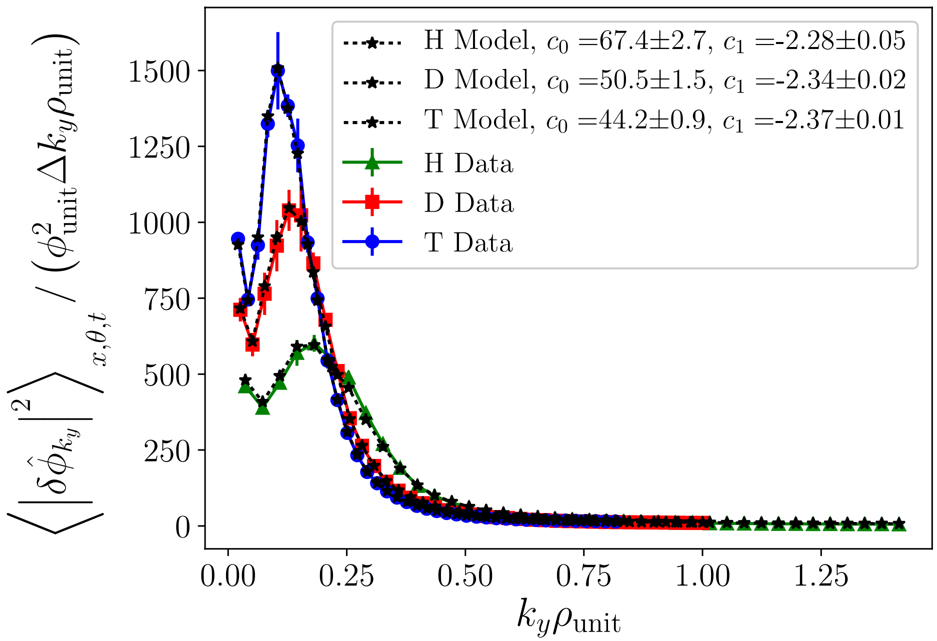
$$= \sum_{k_y>0} \left(\left[\frac{Q^{\delta\phi}_{s,k_y}}{\left\langle\left|\delta\hat{\phi}_{k_y}\right|^2\right\rangle}\right] + \left[\frac{\left\langle\left|\delta\hat{A}_{||,k_y}\right|^2\right\rangle}{\left\langle\left|\delta\hat{\phi}_{k_y}\right|^2\right\rangle}\right]\left[\frac{Q^{\delta A_{||}}_{s,k_y}}{\left\langle\left|\delta\hat{A}_{||,k_y}\right|^2\right\rangle}\right] + \left[\frac{\left\langle\left|\delta\hat{B}_{||,k_y}\right|^2\right\rangle}{\left\langle\left|\delta\hat{\phi}_{k_y}\right|^2\right\rangle}\right]\left[\frac{Q^{\delta B_{||}}_{s,k_y}}{\left\langle\left|\delta\hat{B}_{||,k_y}\right|^2\right\rangle}\right]\right)\left\langle\left|\delta\hat{\phi}_{k_y}\right|^2\right\rangle$$

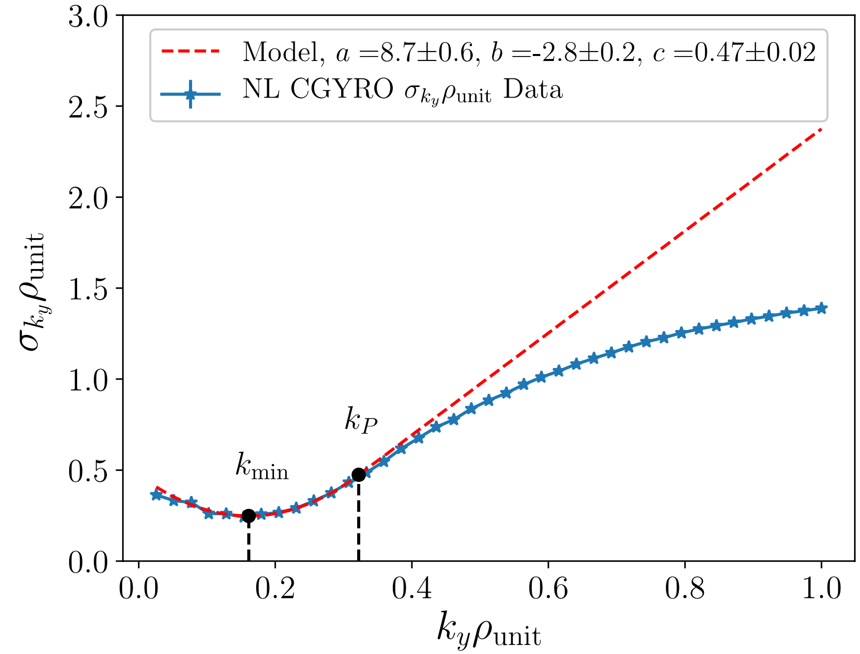
2. Necessity of large databases (e.g. GKDB) and community tools for future saturation rule validation



3. Machine learning approach to linear physics: could offer faster and more accurate linear calculations in well-explored regimes

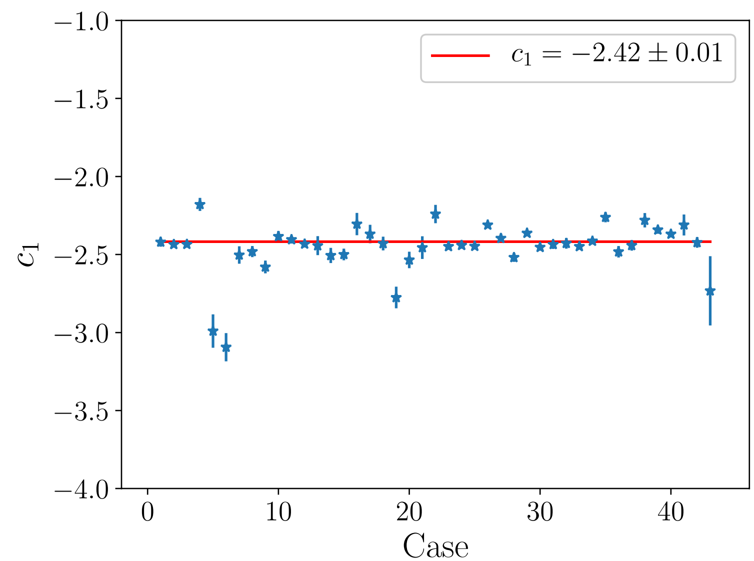
Backup: SAT3 spectral shape





$$\frac{\left\langle \left| \delta\hat{\phi}_{k_y} \right|^2 \right\rangle_{x,\theta,t}}{\Delta k_y} = c_0 \sigma_{k_y}^{c_1}$$

$$\sigma_{k_y} = \begin{cases} a k_y^2 + b k_y + c & 0 < k_y \leq k_P \\ (2 a k_P + b)\, k_y + c - a k_P^2 & k_P < k_y < \infty \end{cases}$$



Backup: Turbulent flux theory

UK Atomic Energy Authority

$$Q_s = 2 \sum_{k_y>0} \sum_{k_x} \frac{k_y}{B_{\mathrm{ref}}} \left\langle \mathrm{Im}\left[\delta\hat{p}^*_{s,k_x,k_y} \delta\hat{\phi}_{k_x,k_y} \right] \right\rangle_{\theta,t}$$

- Turbulent fluxes arise from interactions between:
    - Pressure fluctuations, $\delta\hat{p}^*_{s,k_x,k_y}$
    - Potential fluctuations, $\delta\hat{\phi}_{k_x,k_y}$
- For our purposes, sufficient to write

$$Q_s = \sum_{k_y>0} Q_{s,k_y}$$